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Published in:
Monthly Notices of the Royal Astronomical Society

DOI:
[10.1093/mnras/stu1230](https://doi.org/10.1093/mnras/stu1230)

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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2014

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Latif, M. A., Bovino, S., Van Borm, C., Grassi, T., Schleicher, D. R. G., & Spaans, M. (2014). A UV flux constraint on the formation of direct collapse black holes. *Monthly Notices of the Royal Astronomical Society*, 443(3), 1979-1987. <https://doi.org/10.1093/mnras/stu1230>

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A UV flux constraint on the formation of direct collapse black holes

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Accepted 2014 June 19. Received 2014 June 17; in original form 2014 April 23

ABSTRACT

The ability of metal-free gas to cool by molecular hydrogen in primordial haloes is strongly associated with the strength of ultraviolet (UV) flux produced by the stellar populations in the first galaxies. Depending on the stellar spectrum, these UV photons can either dissociate H_2 molecules directly or indirectly by photodetachment of H^- as the latter provides the main pathway for H_2 formation in the early universe. In this study, we aim to determine the critical strength of the UV flux above which the formation of molecular hydrogen remains suppressed for a sample of five distinct haloes at $z > 10$ by employing a higher order chemical solver and a Jeans resolution of 32 cells. We presume that such flux is emitted by Pop II stars implying atmospheric temperatures of 10^4 K. We performed three-dimensional cosmological simulations and varied the strength of the UV flux below the Lyman limit in units of J_{21} . Our findings show that the value of J_{21}^{crit} varies from halo to halo and is sensitive to the local thermal conditions of the gas. For the simulated haloes, it varies from 400 to 700 with the exception of one halo where $J_{21}^{\text{crit}} \geq 1500$. This has important implications for the formation of direct collapse black holes and their estimated population at $z > 6$. It reduces the number density of direct collapse black holes by almost three orders of magnitude compared to the previous estimates.

Key words: methods: numerical – galaxies: formation – cosmology: theory – early Universe.

1 INTRODUCTION

Observations of quasars at $z > 6$ reveal that supermassive black holes (SMBHs) of a few billion solar masses were assembled within the first billion years after the big bang (Fan et al. 2003, 2006; Willott et al. 2010; Mortlock et al. 2011; Venemans et al. 2013). Their formation mechanisms in the juvenile Universe remain unknown. The potential progenitors of SMBHs include the remnants of Pop III stars (Haiman & Loeb 2001; Haiman 2004; Tanaka & Haiman 2009; Whalen & Fryer 2012; Hirano et al. 2014; Madau, Haardt & Dotti 2014), dense stellar cluster (Portegies Zwart et al. 2004; Omukai, Schneider & Haiman 2008; Devecchi & Volonteri 2009) and direct collapse of a protogalactic gas cloud into so-called direct collapse black holes (DCBHs; Oh & Haiman 2002; Bromm & Loeb 2003a; Begelman, Volonteri & Rees 2006; Lodato & Natarajan 2006; Spaans & Silk 2006; Dijkstra et al. 2008; Djorgovski et al. 2008; Shang, Bryan & Haiman 2010; Schleicher, Spaans & Glover 2010; Volonteri 2010; Johnson et al. 2011; Latif, Zaroubi

& Spaans 2011; Haiman 2012; Volonteri & Bellovary 2012; Aykutalp et al. 2013; Latif et al. 2013c,d,e; Prieto, Jimenez & Haiman 2013; Whalen et al. 2013b; Wutschik, Schleicher & Palmer 2013; Yue et al. 2013, 2014; Inayoshi, Omukai & Tasker 2014; Latif, Niemeyer & Schleicher 2014a; Latif, Schleicher & Schmidt 2014b; Visbal, Haiman & Bryan 2014).

Pristine massive primordial haloes of 10^7 – $10^8 M_\odot$ which formed in the early universe at $z = 15$ – 20 are the potential cradles for these DCBHs. It is imperative that their haloes remain metal free and cooling is mainly regulated by atomic line radiation instead of H_2 . These conditions may lead to a monolithic isothermal collapse where fragmentation is suppressed and a supermassive star of 10^4 – $10^6 M_\odot$ forms which later collapses into a black hole (i.e. DCBH). This scenario is supported by numerical simulations which show that fragmentation remains inhibited and massive objects may form (Bromm & Loeb 2003a; Wise, Turk & Abel 2008; Regan & Haehnelt 2009; Latif, Zaroubi & Spaans 2011; Latif et al. 2013a,b,c). Recently, the feasibility of this scenario has been explored via high-resolution numerical experiments and it is found that $\sim 10^5 M_\odot$ objects can form (Latif et al. 2013e; Regan, Johansson & Haehnelt 2014). These results are consistent with theoretical predictions (Begelman,

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Rossi & Armitage 2008; Begelman 2010; Ball et al. 2011; Ball, Tout & Żytkow 2012; Hosokawa, Omukai & Yorke 2012; Hosokawa et al. 2013; Schleicher et al. 2013; Whalen et al. 2013a). Depending on the mass accretion rates, these studies suggest the formation of supermassive stars or quasi-stars (stars with BH at their centre) as potential embryos of DCBHs (Schleicher et al. 2013).

In primordial gas, trace amount of H_2 can be formed via gas-phase reactions in the early universe which then leads to cooling and star formation. The main channel for the formation of H_2 is



Once the first generation of stars, so-called Pop III stars, are formed, they produce UV flux, pollute the intergalactic medium with metals via supernova explosions and lead to a second generation of stars known as Pop II stars. The UV flux produced by these stellar populations either photodissociates the molecular hydrogen directly or photodetaches electrons from H^- which provides the main route for the formation of H_2 in primordial gas chemistry.

The stellar spectra of Pop III stars are harder with a characteristic temperature of 10^5 K while Pop II stars are characterized by soft spectra with temperatures of 10^4 K. Pop III stars mainly contribute to the direct dissociation of H_2 while Pop II stars also photodetach H^- . UV photons with energies between 11.2 and 13.6 eV are absorbed in the Lyman–Werner bands of molecular hydrogen and put it into an excited state. The H_2 molecule later decays to the ground state and gets dissociated as



a process known as the Solomon process. On the other hand, H^- photodetachment occurs via low-energy photons above 0.76 eV. In this study, we focus on the background UV flux predominantly emitted by Pop II stars as tiny amounts of metals can lead to fragmentation (Omukai et al. 2005; Dopecke et al. 2013).

The critical value of the UV flux, hereafter called J_{21}^{crit} , above which H_2 cooling remains suppressed, can be determined by comparing the H_2 formation and dissociation time-scales. Omukai (2001) found from one-zone calculations that $J_{21}^{\text{crit}} = 10^3$ in units of $J_{21} = 10^{-21} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1} \text{ sr}^{-1}$ for $T_* = 10^4$ K which was later confirmed by Bromm & Loeb (2003b) in 3D simulations for a single halo. These estimates were revised by (Shang et al. 2010, hereafter S10) through three-dimensional simulations using the H_2 self-shielding formula of Draine & Bertoldi (1996), finding that $J_{21}^{\text{crit}} = 30\text{--}300$. They attributed these differences to the choice of a more accurate and higher H_2 collisional dissociation rate, and focused on rather massive haloes forming at $z < 10$. Wolcott-Green, Haiman & Bryan (2011) (hereafter WG11) improved the H_2 self-shielding function of Draine & Bertoldi (1996) and anticipated that it may further reduce the value of J_{21}^{crit} . Such values of J_{21}^{crit} are much larger than the global background flux but can be achieved in the close vicinity (about 10 kpc) of nearby star-forming galaxies (Dijkstra et al. 2008; Agarwal et al. 2012, 2014).

In this paper, we derive the values of J_{21}^{crit} for a stellar spectrum of $T_* = 10^4$ K employing the improved H_2 self-shielding fitting function provided by WG11. Major improvements compared to the previous studies are the following:

- (i) selection of a larger sample of haloes with collapse redshifts at $z > 10$,
- (ii) employed higher order chemical solver DLSODES (Bovino et al. 2013),

- (iii) accurate determination of J_{21}^{crit} for the individual haloes,
- (iv) higher Jeans resolution of 32 cells,
- (v) improved self-shielding function of WG11.

We note that the importance of an accurate chemical solver in high-resolution simulations was previously reported by Bovino et al. (2013). The impact of higher Jeans resolution has also been shown by Latif et al. (2013a) and Turk et al. (2012). Our selected haloes are collapsed at $z > 10$ in contrast to S10 where haloes collapsed at $z < 10$. All these improvements distinguish this work from S10.

We perform three-dimensional cosmological simulations for five different haloes of a few times $10^7 M_\odot$ and vary the strength of the background UV flux (hereafter J_{21} , i.e. UV flux below Lyman limit). We use the chemical network listed in table A1 of S10 which includes all the relevant process for the formation and dissociation of molecular hydrogen. We further employed a fixed Jeans resolution of 32 cells throughout the simulations for better resolving the shocks and turbulence. A particular goal of this paper is to provide a rather narrow constraint on J_{21}^{crit} for individual haloes, and to point at potential correlations with halo properties. This study has important implications for the formation of DCBHs as it provides stronger estimates for the value of J_{21}^{crit} required for dissociation of molecular hydrogen.

The organization of this paper is as follows. In Section 2, we provide the details of simulations setup and summary of a chemical network. In Section 3, we present our findings and discuss our conclusions in Section 4.

2 COMPUTATIONAL METHODS

The simulations presented here are performed using the adaptive mesh refinement, grid-based, cosmological hydrodynamics code ENZO¹ (O’Shea et al. 2004; Bryan et al. 2014). The hydrodynamical equations are solved employing the piece-wise parabolic method and the dark matter (DM) dynamics is computed using the particle-mesh technique. The code makes use of multigrid Poisson solver for solving the gravity.

Our simulations start at $z = 100$ with cosmological initial conditions. We first run 128^3 uniform grid simulations and select the most massive haloes of a few times $10^7 M_\odot$ in our simulated periodic box by using a standard halo finder based on the friends-of-friends algorithm (Turk et al. 2011). Our computational volume has a size of $1 \text{ Mpc } h^{-1}$ and is centred on the most massive halo. We employ two nested refinement levels each with a grid resolution of 128^3 cells besides the top grid resolution of 128^3 . To solve the DM dynamics, 5767 168 particles are used which yield an effective DM resolution of about $600 M_\odot$. Further, additional 18 levels of refinement were employed during the course of the simulations with a fixed Jeans resolution of 32 cells. Our refinement strategy is exactly the same as mentioned in a number of previous studies (Latif et al. 2013c,d, 2014b). For further details about the simulation setup, the reader is referred to the above-mentioned papers. The simulations were stopped once they reached the maximum refinement level, and were performed for five distinct haloes selected from cosmological initial conditions. The masses of these haloes and their collapse redshifts are listed in Table 1 for various values of J_{21} .

To self-consistently solve the evolution of the following chemical species H, H^+ , He, He^+ , He^{++} , e^- , H^- , H_2 , H_2^+ in cosmological simulations, we employed the publicly available KROME package²

¹ <http://enzo-project.org/>, changeset:48de94f882d8.

² Webpage KROME: www.kromepackage.org.

Table 1. Properties of the simulated haloes are listed here.

J_{21}	Mass (M_\odot)	z	$T_{\text{cent}}(\text{K})$	J_{21}	Mass (M_\odot)	z	$T_{\text{cent}}(\text{K})$	J_{21}	Mass (M_\odot)	z	$T_{\text{cent}}(\text{K})$
Halo A				Halo B				Halo C			
300	1.41×10^7	14.24	600	600	2.3×10^7	12.98	700	600	3.22×10^7	11.20	600
600	1.42×10^7	14.23	700	900	2.6×10^7	12.84	1000	700	3.26×10^7	11.11	700
700	1.43×10^7	14.22	7500	1000	2.4×10^7	12.96	1200	900	3.24×10^7	11.13	7500
				1500	2.5×10^7	12.97	1500				
				2000	2.4×10^7	12.93	7500				
Halo D				Halo E							
300	4.06×10^7	13.29	700	300	5.46×10^7	10.60	600				
400	4.08×10^7	13.28	500	500	5.56×10^7	10.549	700				
500	4.08×10^7	13.27	7500	600	5.47×10^7	10.59	7500				
600	4.1×10^7	13.24	7500								

(Grassi et al. 2014). The KROME package was previously employed for 3D simulations of primordial star formation and halo mergers (Bovino et al. 2013, 2014). The chemical network used in this study is the same as listed in table A1 of S10 with only two modifications, the inclusion of an improved fitting formula for H_2 self-shielding by WG11 and an addition of the dissociative tunnelling effect which contributes to the collisional dissociation of H_2 (Martin, Schwarz & Mandy 1996). The latter is the dominant factor in the total dissociation rate ($\gamma_{\text{tot}} = \gamma_{\text{CID}} + \gamma_{\text{DT}}$) of H_2 for temperatures up to 4500 K, see detailed discussion in section 3.3 of Martin et al. (1996). We presume that the background UV flux is emitted by Pop II stars with an atmospheric temperature of $T_* = 10^4$ K.

Here, we are interested in the UV flux below the Lyman limit (i.e. < 13.6 eV). As pointed out in the previous section, the low-energy photons with energy above 0.76 eV emitted by Pop II stars photodetach H^- which provides the main pathway for the formation of H_2 in primordial composition of the gas. We have not included the photoionization of hydrogen and helium species as they require energies above the Lyman limit. The H_2 cooling function of Galli & Palla (1998) is used here as in S10 for direct comparison and all other relevant cooling processes for primordial gas are included, i.e. cooling by collisional excitation, collisional ionization, recombination and Bremsstrahlung radiation (for details, see Grassi et al. 2014). We checked that using the cooling function by Glover & Abel (2008) has no impact on the results.

3 MAIN RESULTS

3.1 Results from one-zone models

To test our chemical model, we have performed one-zone calculations similar to S10. The thermal evolution and species fractions of H_2 , H^- and e^- are shown in Fig. 1. We start with an initial density of 1 cm^{-3} , a gas temperature of 200 K, electron and H_2 fractions of 10^{-4} and 10^{-10} , respectively (same as S10). It can be seen from Fig. 1 that for $J_{21} < 30$, H_2 formation takes place and leads to cooling down to a few hundreds K. The H^- fraction initially increases up to densities of 100 cm^{-3} , then gets depleted during the formation of H_2 . For stronger fluxes, the formation of H_2 remains inhibited, cooling due to Lyman alpha photons kicks in and the temperature remains about 8000 K. The thermal evolution and the abundances of the species are in agreement with S10. The value of J_{21}^{crit} found from one-zone calculations is between 30 and 40 and is consistent with findings of S10.

However, we note that the value of J_{21}^{crit} differs in 3D simulations. The differences in J_{21}^{crit} between one-zone and three-dimensional

simulations arise from the fact that the one-zone calculation do not capture shocks, collapse dynamics, hydrodynamical effects as well as the effects of the DM potential which are crucial in determining the J_{21}^{crit} .

3.2 Results from 3D simulations

To determine J_{21}^{crit} , we have performed more than 20 cosmological simulations for five distinct haloes with masses above $10^7 M_\odot$ including all the necessary processes for the formation and dissociation of molecular hydrogen by self-consistently solving the rate equations along with the hydrodynamics. In Fig. 2, we present the spherically averaged profiles of temperature, density, H_2 and e^- abundances for all simulated haloes. It is found that in all haloes the formation of H_2 takes place for $J_{21} < 300$. At radii $> 2 \times 10^5$ au, the temperature in all cases for the various strengths of J_{21} is about 7500 K but the fraction of the molecular hydrogen remains higher for the lower values of J_{21} . This is because the H^- photodetachment rate scales linearly with the strength of J_{21} , i.e. the stronger the flux, the lower the fraction of molecular hydrogen. For fluxes below the critical values, the fraction of H_2 gets further boosted during the collapse and reaches $\sim 10^{-3}$. It cools the gas down to temperatures of about 1000 K. Similarly, the electron fraction declines towards the centre. It is about 10^{-7} in the centre and 10^{-4} at larger radii. The impact of H_2 cooling is also visible in the density profile which significantly deviates from the isothermal profile. Small bumps in the density profile are typical signatures of fragmentation which is expected in these cases. This trend is observed in all the haloes for $J_{21} = 300$.

For some haloes, the fraction of H_2 sufficient to induce cooling still occurs at later times for $J_{21} > 300$, at densities of about 10^5 cm^{-3} . This lowers the halo central temperatures down to about 1000 K. For J_{21} above the critical threshold, the fraction of H_2 remains quite low, i.e. 10^{-8} . Such a low fraction is not sufficient to trigger H_2 cooling and then the haloes collapse isothermally. We note that value of the J_{21}^{crit} varies from 400 to 700 for four haloes as listed in Table 2. A notable variation in the critical value is observed for halo B where $J_{21}^{\text{crit}} = 1500$. Such variations from halo to halo are not surprising as haloes have different density distributions after virialization, different spins and accretion shocks at different densities. As shown in figs 6 and 7 of S10, collisional dissociation is the main destruction channel for H_2 above densities of 10^3 cm^{-3} . The rate of collisional dissociation exponentially depends on the temperature (Martin et al. 1996), and small local variations in the temperature can change J_{21}^{crit} as verified from our one-zone model by artificially changing the temperature by a few hundreds K.

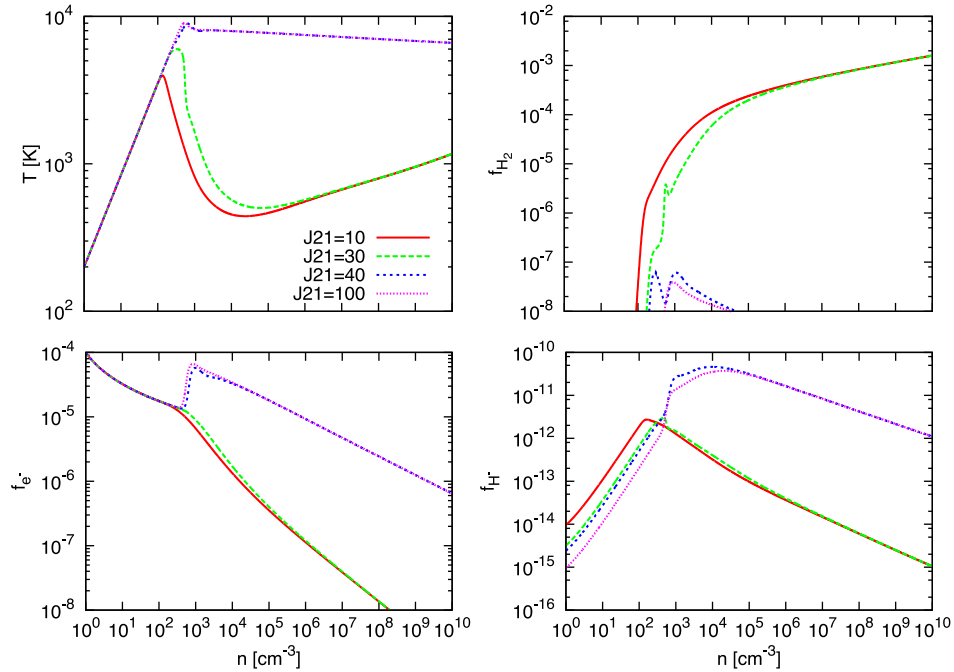


Figure 1. The abundances of H_2 , e^- , H^- and temperature are plotted against the number density for various strengths of background UV flux. These results are one-zone calculations performed using the H_2 self-shielding function of Draine & Bertoldi (1996).

Additional fluctuations in the electron number density may further influence it and there is a weak dependence of the collisional dissociation on density as well. As these quantities change simultaneously when different haloes are considered, the individual dependences cannot be explored in isolation, but the functional form of collisional dissociation rate suggests that temperature dependence provides the dominant effect (also see discussion in S10).

In Fig. 3, we show the phase plots of temperature and H_2 fraction against density. Initially, the gas is heated up to the virial temperature of the halo, i.e. above 10^4 K , and then cools down to about 8000 K by Lyman alpha radiation. At densities of about 10^4 cm^{-3} , cooling due to H_2 becomes effective for the weaker J_{21} case while for the stronger flux case it remains inhibited. It is found that temporarily different gas phases may coexist at the same density. The latter reflects local variations in gas density, temperature and self-shielding. It may also be noted that in the latter case, the amount of gas in the cold phase is negligible compared to the top panel which has a significant amount of cold gas and remains in the cold phase. In these simulations, we find that if the gas at densities $\geq 10^3 \text{ cm}^{-3}$ has a temperature lower than 1000 K (as shown in top panel of Fig. 3) then cooling due to H_2 becomes important and haloes remains in cold phase. On the other hand, if gas at densities $\geq 10^3 \text{ cm}^{-3}$ has a temperature higher than 2000 K shown in the bottom panel of Fig. 3, then the halo remains in the hot phase and collapses isothermally. We have also checked that the behaviour remains the same if the simulations are evolved to higher densities.

To further understand the origin of J_{21}^{crit} , we have plotted the radially averaged density, temperature, abundances of H_2 and e^- , radial infall velocities as well as rotational velocities of all haloes for $J_{21} = 600$ in Fig. 4. For the given strength of J_{21} , two haloes (D and E) are already in an isothermal state with central temperature around 7000 K while the other three have a sufficient H_2 fraction to reduce their central temperatures down to about 1000 K . It can be noted that particularly haloes D and E have larger infall velocities already at radii $> 10^5 \text{ au}$ compared to the haloes with lower central

temperatures. Particularly, the halo B with the highest J_{21}^{crit} in our sample has the lowest infall velocity. The differences in the infall velocities arise due to the ambient sound speed of gas cloud. We further note that the two most massive haloes have a lower value of J_{21}^{crit} than the lower mass haloes. S10 have considered even more massive haloes at lower redshift, finding a further decrease in J_{21}^{crit} . The latter suggests a potential dependence on the mass of the halo with some fluctuations.

3.3 Comparison with previous studies

For a comparison of our results with S10, we have performed a couple of simulations where we employed exactly the same chemical and thermal processes as described by S10 without any modifications and using the H_2 self-shielding fitting function of Draine & Bertoldi (1996). These simulations were performed for haloes C and D and are shown in Fig. 5. It suggests that the value of J_{21}^{crit} differs by a factor of a few from their estimates as they suggest that J_{21}^{crit} varies from 30 to 300. Our study brackets the value of J_{21}^{crit} within a factor of 2. The self-shielding fitting function of Draine & Bertoldi (1996) is known to overestimate the H_2 shielding. Therefore, a more accurate determination of J_{21}^{crit} is not necessary. In addition, we found significant variations from halo to halo as well. Given the strong dependence of J_{21}^{crit} on the variations in the local gas temperatures, halo merger histories, the occurrence of shocks at various densities as well as the density and temperature dependence of the H_2 collisional dissociation rates, the results may still be consistent with S10, even though we typically obtain higher values for the J_{21}^{crit} . Variations in the temperature and the occurrence of the shocks is evident from Fig. 3. As mentioned in previous section, we further verified it by artificially changing the temperature in our one-zone model. This was already confirmed by S10 as well (see paragraph 2, section 3.5 of S10). It may also be noted that the haloes in our sample are assembled at higher redshifts and have lower masses compared to

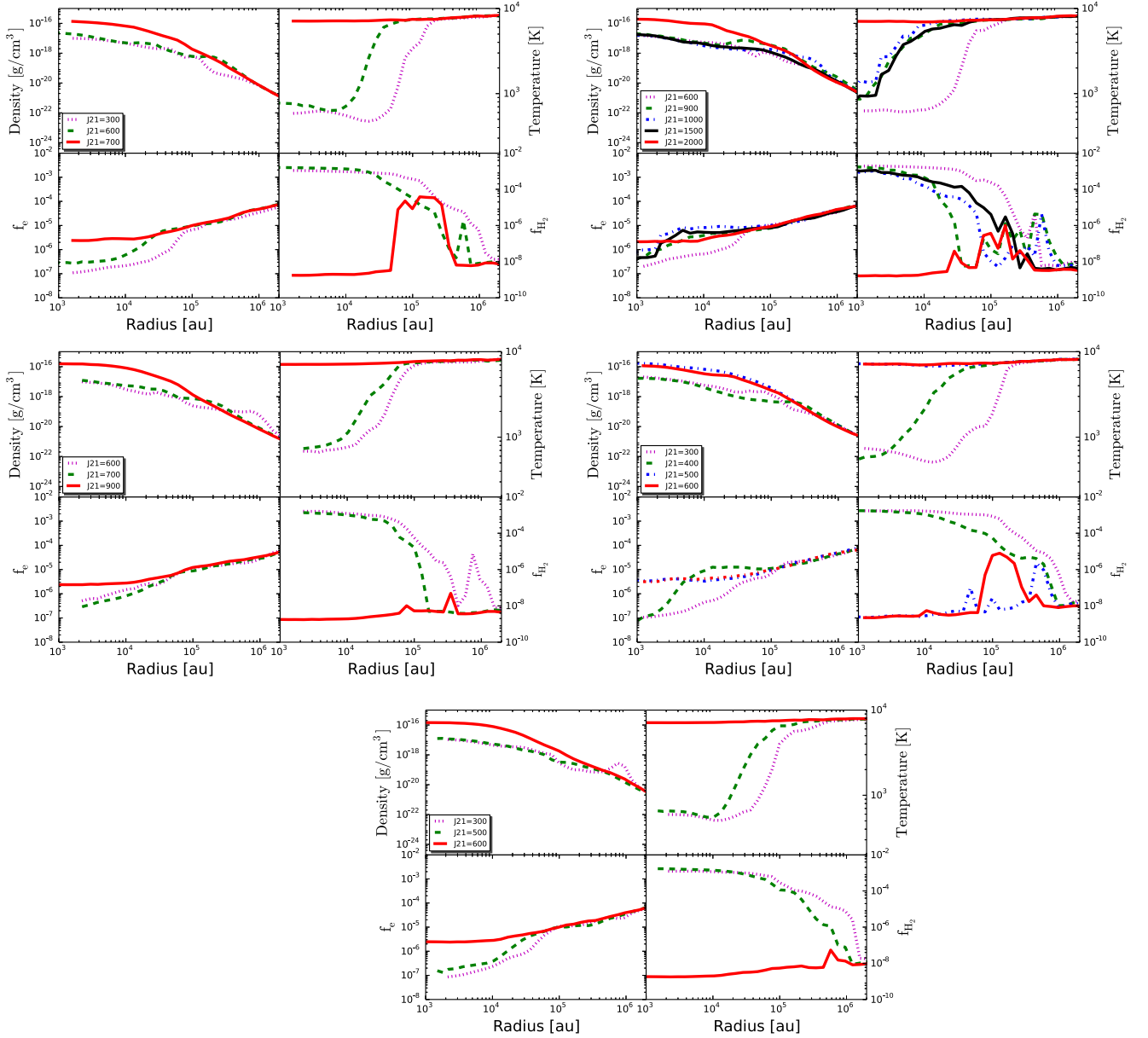


Figure 2. Spherically averaged and radially binned profiles of temperature, density, H₂ and e[−] fractions are plotted in this figure. Each panel represents a single halo. Each line style represents the value of J_{21} as mentioned in the legend. Top panels represent halo A and B (left to right), middle panels haloes C and D (left to right) and bottom panel halo E.

Table 2. Properties of the simulated haloes for J_{21}^{crit} are listed here.

Model no.	Mass (M_{\odot})	Redshift z	J_{21}^{crit} in units of J_{21}	Spin parameter λ
A	1.42×10^7	14.23	600	0.025
B	2.4×10^7	12.95	1500	0.009
C	3.25×10^7	11.11	700	0.03
D	4.06×10^7	13.29	400	0.02
E	5.6×10^7	10.55	500	0.034

the S10, and therefore presumably different structures as well as formation histories.

We further noted that the value of J_{21}^{crit} very weakly depends on the choice of self-shielding function. It is due to the fact that for a stellar temperature of $T_* = 10^4$ K the main dissociation channel is

H[−] photodetachment not the direct dissociation of H₂. The value of J_{21}^{crit} changes within a factor of 2 at most by employing the self-shielding fitting function of Draine & Bertoldi (1996) which overestimates the shielding effect. S10 also found similar results (Haiman, private communication).

3.4 Implications for the formation of DCBHs

The key requirements for the formation of DCBHs are that the gas in haloes with $T_{\text{vir}} > 10^4$ K must be of primordial composition and the formation of molecular hydrogen remains suppressed to avoid fragmentation. To keep the gas free from H₂ requires the presence of a strong UV flux above the critical value. Such values of J_{21}^{crit} can be achieved in the surrounding of starburst galaxies or even in the haloes which are satellites of such galaxies (Dijkstra et al. 2008;

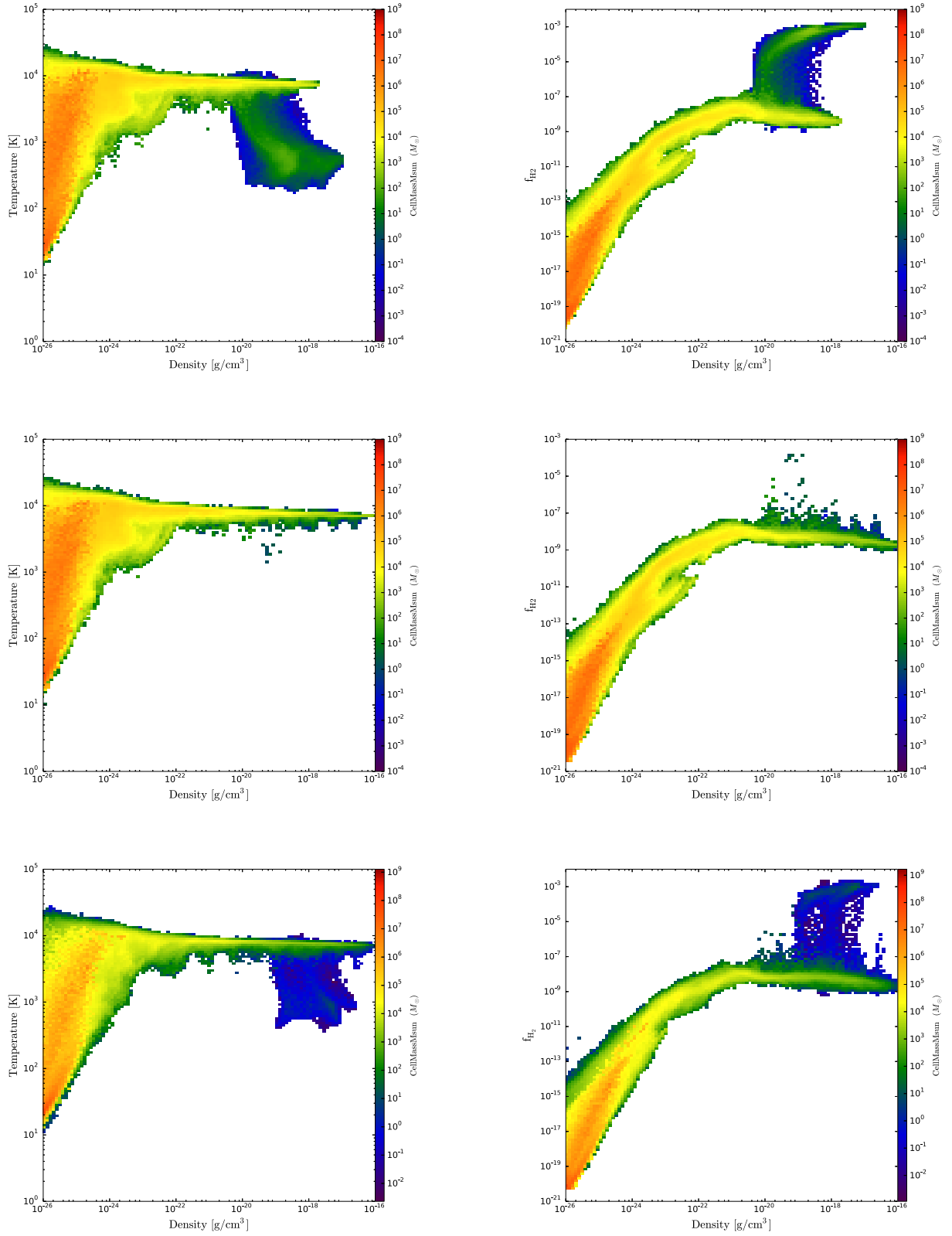


Figure 3. Phase plots of temperature, density and H₂ fraction for representative cases of haloes E and D are shown here. The top panel shows $J_{21} = 300$ for halo E, the middle panel $J_{21} = 600$ for the halo E and the bottom panel $J_{21} = 600$ for the halo D. The latter case also illustrates the existence of two gas phases at the same density.

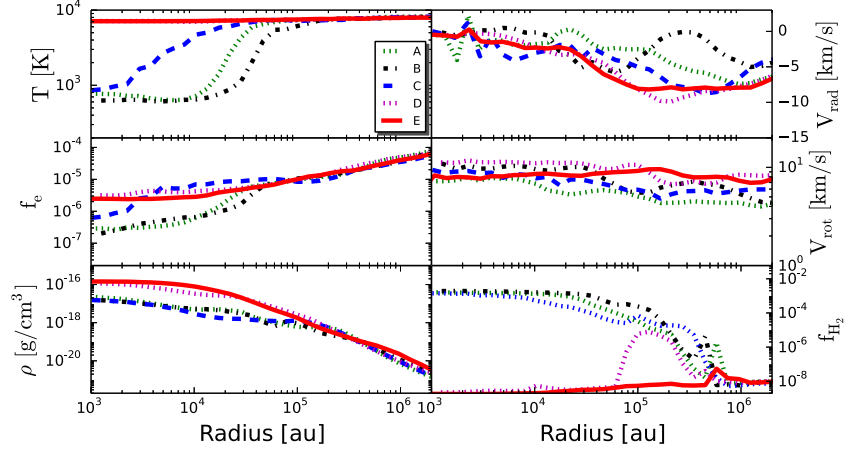


Figure 4. Spherically averaged and radially binned profiles of temperature, density, H₂ fraction, e⁻ fraction, radial infall velocity and rotational velocities are plotted for all haloes for $J_{21} = 600$.

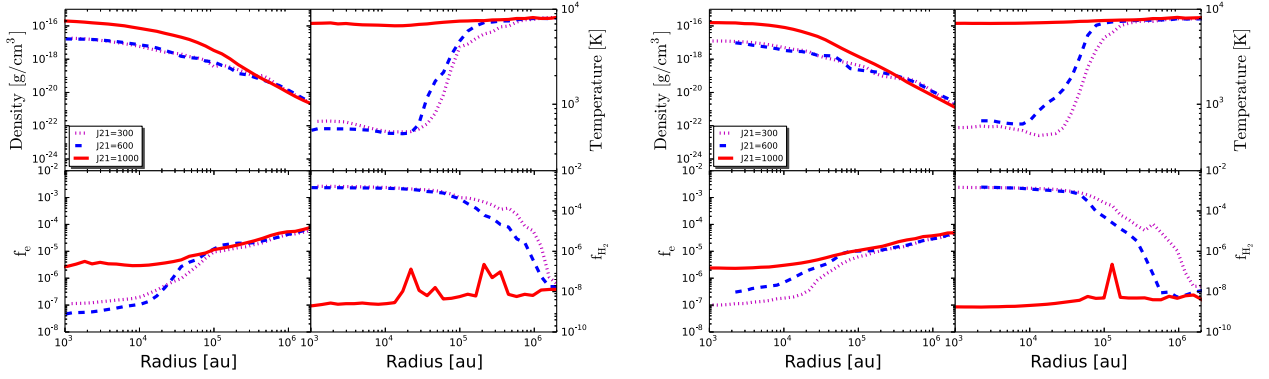


Figure 5. Same as Fig. 2 for halo D and C but using the H₂ self-shielding fitting function of Draine & Bertoldi 1996.

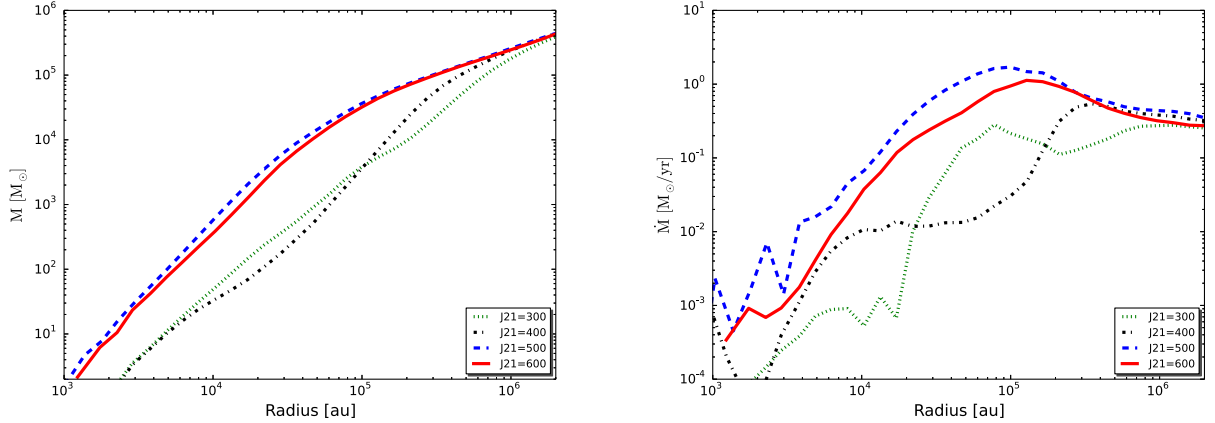


Figure 6. Enclosed masses and mass accretion rates are shown for a representative case of ‘halo D’. The left-hand panel shows enclosed mass profiles while the right-hand panel shows the mass accretion rates.

Agarwal et al. 2012, 2014). We have computed the enclosed mass and mass accretion rates for halo ‘D’ as a representative case which is shown in Fig. 6. It is found that for an isothermal collapse, the gas in the halo remains hotter, leads to higher accretion rates and consequently the enclosed mass within 10^5 au is about two orders of magnitude higher compared to the case with the weaker UV flux. The mass accretion rate peaks around $1 M_{\odot} \text{ yr}^{-1}$ for isothermal cases and overall is about an order of magnitude higher compared to the H₂ cooling cases. One may expect similar differences in the

mass of resulting objects. These enhanced accretion rates help in rapidly building up the DCBHs.

Our estimates of J_{21}^{crit} are highly relevant for computing the number density of DCBHs and their comparison with observations. Some recent studies predict the number density of DCBHs of few per comoving Mpc^{-3} compared to the observed SMBHs density of few per comoving Gpc^{-3} (Dijkstra et al. 2008; Agarwal et al. 2012). Our results suggest that for the most of haloes simulated in these studies, $J_{21}^{\text{crit}} \geq 400$. The choice of such critical values changes the

number density of DCBHs and also helps these models to have better agreement with observations. Based on the prescription for estimating the fraction of haloes exposed to supercritical UV flux by Dijkstra et al. (2008) and Agarwal et al. (2012), we estimate that fraction of the haloes hosting DCBHs may be reduced by about three orders of magnitude due to the increase in J_{21}^{crit} by an order magnitude, i.e. adapting $J_{21}^{\text{crit}} = 400$. The expected number density of BHs is 10^5 per comoving Gpc^{-3} at $z = 6$. The latter is still a factor of 500 or so higher than observed number density. These estimates do not include the metal enrichment by supernova-driven winds (see Dijkstra et al. 2008 and Agarwal et al. 2012) which will further reduce the number density of DCBHs. We also report here a potential mass dependence of J_{21}^{crit} , which tends to increase with decreasing halo mass. In order to give black holes more time to accrete, the initial collapse should take place at higher redshift, at a virial temperature of 10^4 K. The latter implies a decreasing mass for higher redshift DM haloes, corresponding to a higher value of J_{21}^{crit} .

4 DISCUSSION

One of the main obstacles for the formation of DCBHs is to avoid fragmentation in massive primordial haloes which are the potential birthplaces of seed black holes. This may only be possible in the absence of molecular hydrogen which may induce fragmentation and trigger star formation. The ubiquity of background UV flux can photodissociate H_2 molecules and may overcome this obstruction. The prime objective of this work is to determine the critical value of the background UV flux required to suppress the molecular hydrogen formation in atomic cooling haloes. As photodissociation of H_2 depends on the type of stellar spectrum, we have considered here UV photons below 13.6 eV emitted by Pop II stars. We have conducted three-dimensional cosmological simulations for five distinct haloes by including all relevant processes for the formation and dissociation of H_2 . The haloes studied here have typical masses of a few times $10^7 M_\odot$ and were illuminated by various strengths of background UV flux. We here employed the H_2 self-shielding fitting function provided by WG11.

Our findings show that the value of J_{21}^{crit} strongly depends on the properties of the halo and may vary from halo to halo. For the haloes studied here, we found that the value of J_{21}^{crit} varies from 400 to 700 with the exception of one halo where it is about 1500. It is also found that J_{21}^{crit} may depend on the mass of halo, as the two most massive haloes have reduced values of J_{21}^{crit} . This trend is consistent with results by S10, where more massive haloes have even lower values of J_{21}^{crit} . We note that our one-zone calculations are in agreement with S10. The highly non-linear collapse dynamics leads to the occurrence of shocks with Mach numbers of about 3 at various densities which changes the local gas temperature and consequently J_{21}^{crit} differs from halo to halo due to the strong dependence of H_2 collisional rate on temperature and density (Martin et al. 1996). To build up the SMBHs at $z = 6-7$, one should preferentially consider haloes that collapse early, implying a lower mass and potentially higher J_{21}^{crit} at the same virial temperature. However, it will be desirable in the future to verify it for a larger sample of haloes with broader mass range. Our estimates for J_{21}^{crit} are quite robust as we consider a larger sample of haloes and higher Jeans resolution leading to better resolved shocks and employed the high-order chemical solver DLSODES. We also find that the value of J_{21}^{crit} weakly depends on the choice of H_2 self-shielding. Although, the fitting formula of Draine & Bertoldi (1996) overestimates H_2

self-shielding compared to WG11, its impact is very low for the adapted stellar spectra.

The value of J_{21}^{crit} is about an order of magnitude higher in 3D calculations compared to the one-zone results. This is because of the inability of one-zone calculations to model shocks and hydrodynamical effects. Similar results have been found in the study of S10. We also included the effect of dissociative tunnelling and found from the one-zone test that it decreases J_{21}^{crit} by a factor of 3. The estimates of J_{21}^{crit} determined in this work have important implications for the formation of DCBHs. Our results suggest that the value of $J_{21}^{\text{crit}} > 400$ should be employed in computing the number density of DCBHs. The value of J_{21}^{crit} used in previous studies (Agarwal et al. 2012, 2014) seems rather low (i.e. 30) and may be one of the reasons for the high abundance of DCBHs predicted from semi-analytical calculations. From our results, the expected BH number density is 10^5 per comoving Gpc^{-3} at $z = 6$ for $J_{21}^{\text{crit}} = 400$. This estimate is obtained by rescaling the values of (Agarwal et al. 2012) for a higher J_{21}^{crit} . These estimates do not take into account the metal enrichment in the intergalactic medium by supernova-driven winds which may further reduce the number density of DCBHs.

In our previous studies (Latif et al. 2013c,e, 2014a), we have shown that the presence of strong UV flux leads to an isothermal collapse where conditions are fertile for the formation of DCBHs. In fact, under these conditions, large accretion rates of $> 1 M_\odot \text{yr}^{-1}$ are observed which result in the formation of supermassive stars of $10^5 M_\odot$, the potential progenitors of DCBHs.

We have presumed here that these haloes exposed to the intense UV flux by Pop II stars are metal free and remain pristine throughout their evolution. The transition from Pop III to Pop II stars may inject metals and pollute these haloes. Depending on the critical value of metallicity which can be as low as $10^{-5} Z/Z_\odot$ (Cazaux & Spaans 2009; Aykutalp & Spaans 2011; Latif, Schleicher & Spaans 2012), once the metal content in haloes exceeds this value fragmentation becomes inevitable (Omukai et al. 2008). Particularly, the cooling due to the dust even in the presence of a strong UV flux becomes effective at densities around $10^{12}-10^{15} \text{cm}^{-3}$ and may lead to the formation of dense stellar clusters (Devecchi & Volonteri 2009). Nevertheless, metal enrichment in the universe is expected to be patchy and pristine haloes may exist down to $z > 6$.

Given the strong dependence of J_{21}^{crit} on the local thermal conditions as argued above, the local heating/cooling effects such as heating by ambipolar diffusion, turbulence dissipation as well as cooling by HD molecules may change the critical value of the flux by a factor of few. In fact, the impact of turbulence and magnetic field in the presence of UV flux was explored by Van Borm & Spaans (2013) and they found that in turbulent haloes with stronger initial seed fields the value of J_{21}^{crit} is reduced by an order of magnitude. Furthermore, the presence of cosmic rays/X-rays may significantly enhance the critical value of J_{21} (Inayoshi & Omukai 2011). It was recently pointed out by Richings, Schaye & Oppenheimer (2014) that including the effect of turbulence in Doppler broadening reduces the H_2 self-shielding. This should be explored in future studies.

ACKNOWLEDGEMENTS

The simulations described in this work were performed using the ENZO code, developed by the Laboratory for Computational Astrophysics at the University of California in San Diego (<http://lca.ucsd.edu>). We thank Zoltan Haiman and Greg Bryan for useful discussions on the topic. We acknowledge research funding by Deutsche Forschungsgemeinschaft (DFG) under grant SFB

963/1 (project A12) and computing time from HLRN under project nip00029. DRGS and SB thank the DFG for funding via the Schwerpunktprogramm SPP 1573 “Physics of the Interstellar Medium” (grant SCHL 1964/1 – 1). The simulation results are analysed using the visualization toolkit for astrophysical data YT (Turk et al. 2011).

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